

Description of Additional Supplementary Files

Supplementary Movie 1: Video clip illustrating the steps of AIMD simulation, showcasing the perturbation of atom positions in Ba-free $\text{NbIr}_3\text{O}_{12}\text{H}_8$ of the $\text{Ba}_4\text{NbIr}_3\text{O}_{12}$ framework.

Supplementary Data 1: Files for the atomic coordinates of the optimized unit cell and the initial and final configurations of AIMD simulation.